國立台灣科技大學九十六學年度碩士班招生試題

系所組別： 化學工程系碩士班

科　　目： 化工熱力學與動力學

總分100分

Part I. 化工熱力學 (50%)

(1) Derive the Clapeyron equation that relates the slope of the vapor-liquid coexistence curve to the enthalpy and volume changes at phase transition. (15%)

(2) An adiabatic compressor is used to compress air (an ideal gas) from 1 bar and 290 K to 10 bar and 575 K. What is the value of $\triangle S$ (entropy change) for this process? How much work per mole of air ($\underline{W}_s$) is needed for the compression process? Data: C_p = 29.3 J mol^{-1} K^{-1}, R = 8.314 J mol^{-1} K^{-1}. (10%)

(3) For a fluid that follows the relationship P ($\underline{V}$ − b) = R T, where b is a constant, derive expressions for the Gibbs free energy departure function $(\underline{G} - \underline{G}^{IG})_{T,P}$ and fugavity (f) of this fluid, respectively. Determine the fugacity of this fluid if the pressure is 1 atm and the compressibility factor is 0.9. (15%)

(4) Consider 5 kg of steam contained within a piston-cylinder assembly. The steam undergoes an expansion from state 1 ($\mathbf{U}_1$ = 2709.9 kJ kg^{-1}) to state 2 ($\mathbf{U}_2$ = 2659.6 kJ kg^{-1}). During the process, there is a heat transfer of energy to the steam with a magnitude of 80 kJ. Also, a paddle wheel transfers energy to the steam by work in the amount of 18.5 kJ. Determine the amount of energy transfer by work from the steam to the piston during the process. (10%)

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Part II. 化工動力學

1. (25%)

An elementary gas-phase reaction

$$A \rightarrow B + C$$

is carried out isothermally at 127°C in a flow reactor with no pressure drop. The specific reaction rate at 127°C is 0.044 min^{-1}. Pure A enters the reactor at 10 atm and 127°C and a molar flow rate of 2.5 mol/min. Calculate the reactor volume and space time to achieve 90% conversion in:

(a) a continuous-stirred tank reactor (CSTR) (10%)

(b) a plug-flow tubular reactor (PFR) (10%).

(c) Assume that the reaction is reversible with $K_C = 0.11$ mol/dm^3, calculate the equilibrium conversion, X_e. (5%)

Hint: Useful formula for this problem

(1) $\int_0^x \frac{1+\varepsilon x}{1-x} dx = (1+\varepsilon) \ln \frac{1}{1-x} - \varepsilon x$

(2) The five-point quadrature formula for the integration $\int_{x0}^{x4} f(x)dx = h/3(f_0+4f_1+2f_2+4f_3+f_4)$,

where f_i is the function value at x_i, and $h = (x_4-x_0)/4$

(3) For $ax^2 + bx + c = 0$, the roots, p and q, are $\frac{-b \pm \sqrt{b^2-4ac}}{2a}$

Show All Your Work.

2. (15%)

Pharmacokinetics (藥物動力學) concerns the ingestion (攝取), distribution, reaction, and elimination (移除) reaction of drugs in the body. Consider the application of pharmacokinetics to one of the major problems in Taiwan, drinking and driving (酒醉開車). Here, we shall model how long one must wait to drive after having a tall martini (一高杯的馬丁尼酒). In Taiwan, the legal intoxication limit (法定酒醉限值) is 0.53 g of ethanol (酒精) per liter of body fluid. (In the United States, it is 0.8 g/L, in Sweden it is 0.5 g/L, and in Eastern Europe and Russia it is any value above 0.0 g/L.) The ingestion of ethanol into the bloodstream(血液) and subsequent elimination can be modeled as a series reaction. The rate of absorption from the gastrointestinal tract (腹部的腸道) into the bloodstream and body is a first-order reaction with a specific reaction rate constant of 10 h^{-1}. The rate at which ethanol is broken down in the bloodstream is limited by regeneration of a coenzyme. Consequently,

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the process may be modeled as a zero-order reaction with a specific reaction rate of 0.192 g/h·L of body fluid.

(a) How long would a person have to wait to drive in Taiwan if they drank two tall martinis immediately after arriving at a party? (10%)

(b) Suppose that one went to a party, had one and a half tall martinis right away, and then received a phone call saying an emergency had come up and the person needed to drive home immediately. How many minutes would the individual have to reach home before he/she became legally intoxicated (超出法定酒醉限值), assuming that the person had nothing further to drink? (5%)

(Hint: Base all ethanol concentrations on the volume of body fluid. Calculate and plot the concentration of ethanol in the blood as a function of time.)

Additional information:

Ethanol in a tall martini: 40 g

Volume of body fluid: 40 L

Show All Your Work.

3. (10%)

Titanium dioxide is a wide-bandgap semiconductor that is showing promise as an insulating dielectric in VLSI capacitors and for use in solar cells. Thin films of TiO_2 are to be prepared by *chemical vapor deposition* from gaseous titanium tetraisopropoxide (TTIP). The overall reaction is

$$Ti(OC_3H_7)_4 \rightarrow TiO_2 + 4C_3H_6 + 2H_2O$$

The reaction mechanism in a CVD reactor is believed to be

$$TTIP(g) + TTIP(g) \Leftrightarrow I + P_1$$
$$I + S \Leftrightarrow I{\cdot}S$$
$$I{\cdot}S \rightarrow TiO_2 + P_2$$

where I is an active intermediate and P_1 is one set of reaction products (e.g., H_2O, C_3H_6) and P_2 is another set. Assuming the homogeneous gas-phase reaction for TTIP is in equilibrium, derive a rate law for the deposition of TiO_2.

The experimental results show that at 200°C the reaction is second order at low partial pressures of TTIP and zero order at high partial pressures, while at 300°C the reaction is second order in TTIP over the entire pressure range. Discuss these results in light of the rate law you derived.

Show All Your Work.